CHEMISTRY AND MATERIALS SCIENCE

Providing scientific excellence and leadership that meets and anticipates the needs of the Laboratory's programs

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Message from the Associate Director

In September, the CMS management team presented our FY05 budget and investment strategy to the Laboratory. Our message was unambiguous: We continue to make sustained, multiyear investments in areas that are strongly aligned with our strategic plan and with the Laboratory's long-range S&T plan.

New Initiatives

In the past year, we have seen rapid growth of external funding for several startup efforts, particularly the BioSecurity and Nanosciences Laboratory (BSNL) and the Glenn T. Seaborg Institute. With the strong involvement of multiple directorates and innovative scientific breakthroughs, both have transformed themselves from modest initiatives to critical components of the Laboratory's core mission.

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Corner on Science

Focus on a New Laboratory



Technician Nick
Teslich, a descendent of inventor
Nikola Tesla, operates the focused ion beam in the
Nanobeam Precision
Characterization
Laboratory.

In the basement of Building 235, the Nanobeam Precision Characterization Laboratory is just now opening its doors. Under the direction of Art Nelson and Mark Wall, this clean-room facility has two instruments that allow Lab scientists to characterize and fabricate materials with nanometer resolution.

The first to come online is the focused ion beam (FIB), a tool that combines an imaging electron beam and

an ion beam to either remove or add miniscule bits of material. Recently hired technician **Nick Teslich** is operating the FIB. The other instrument will be a high-resolution scanning transmission electron microscope (STEM) known as a SuperSTEM. An interim version of the SuperSTEM will arrive toward the end of this year, and the final instrument—the most powerful of its kind—will be in place in 2006.

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Interview With...

Pat Allen

Recruiting, strategic planning, mentoring LDRD projects, handling the occasional performance management challenge—such is the daily routine of **Pat Allen**.

As deputy division leader for science and technology in CChED, Pat is responsible for all of these tasks and more.

One of his favorite activities is brainstorming about what the new S&T thrusts should be for extreme chemistry and material synthesis. Pat helped frame and write the "Chemistry Under Extreme Conditions" portion of CMS's recently published *Strategic Plan* and is pleased to

have the document in place. "However," he notes, "now we have to implement it!"

Another favorite job is recruiting, finding the best talent from top universities around the world. Most of his recruiting is for chemical engineers and scientists, especially

optical materials specialists, to meet the needs of the National Ignition Facility. As most of us know, NIF is not only the largest laser in the world, but it is also the world's largest optical instrument.

The newly formed NIF Recruiting Action Team, which Pat leads, has found that their most effective tool for reaching top graduates is targeted recruiting. CMS staff maintain contacts with former men-

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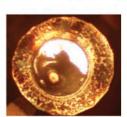


Notable Publications BY MICHAEL FLUSS

Scientists Pressured to Succeed

Livermore scientists working with collaborators from across the country are reporting on experiments and modeling showing that petroleum and other fuels are formed by purely chemical, or abiogenic, processes hundreds of miles inside the Earth. Their results appeared in the September 20 issue of the Proceedings of the National Academy of Sciences. One objection to the theory of abiogenic fuels is that they would quickly disintegrate in the extreme heat and pressure hundreds of miles beneath the surface. But the team's experiments show that methane gas can remain chemically stable at pressures and temperatures similar to those some 120 to 180 miles beneath the surface. The scientists created a microsimulation inside a diamond anvil cell of the presumed mineral composition of the deep Earth, squeezing iron oxide, calcium carbonate, and water together at pressures many thousands of times the pressure of Earth's atmosphere. The mixture was heated with a laser up to 2,700° F, producing methane. On this basis, Livermore members of the team calculated that the methane "could be stable for millions of years." The article's authors include Larry Fried and Michael Howard of CMS, Sorin

Bastea of the Physics and Applied



Technologies
Directorate,
and researchers
from Indiana
University,
the Carnegie
Institution,
and Harvard

Methane was formed in a diamond anvil cell, in a sample crushed to about 100,000 times atmospheric pressure.

University. ■
Publication URLs:
http://www.pnas.org/cgi/content/full/
101/39/14023
http://www.nature.com/news/2004/
040913/full/040913-5.html

Chemists Reveal Solid Background

A research group led by Joe Zaug has been exploiting its success in deducing the bulk properties of solids by impulsive stimulated light scattering (ISLS). Two papers on this work have appeared recently. The article in Physical Review Letters 91 (11) was written by CMS scientists Alexander F. Goncharov, Jonathan Crowhurst, and Zaug. In this work, ISLS and Raman spectroscopy measurements were made on hcp cobalt to a static pressure of 120 GPa. The researchers found that at pressures above 60 GPa, the shear elastic modulus and the Raman frequency of the E2g transverse optical phonon exhibit a departure from a linear dependence on density. They relate this behavior to a collapse of the magnetic moment under pressure that has been predicted theoretically but until now not observed experimentally. They also note the possibility for unconventional superconductivity usually only seen in complex ternary systems consisting of 4f or 5f electron materials. A second paper by two team members (Crowhurst and Zaug) was also published recently in Physical Review B. Here, they used ISLS to measure surface wave power spectra of germanium single crystals and reported a significant improvement in experimental technique. The observed power spectra contained sufficient information to determine all the elements of the elastic tensor with a high degree of spectral resolution and in relatively short measuring times.

Publication URLs: Physical Review Letters 91 (11): http://prl.aps.org/ Physical Review B 69 (5), Article 052301: http://prb.aps.org/

Please send items for the next newsletter (e.g., directorate news, awards, conference calendar items) to **Stephanie Shang** (shang2@llnl.gov). Fall 2004



CMS Team News

Meet the CMS Facility Operations Team: They Keep It All Humming

Need your lab remodeled? Planning an office move? Discovered a toilet not working properly? Who're you going to call? The CMS facility operations team!

CMS facility manager Carey Bailey has responsibility for 14 CMS buildings at the Livermore site, while his counterpart at Site 300, John Scott, manages over 50 buildings and storage magazines. Carey, John, and their teams oversee more than 500,000 square feet of offices, laboratories, and storage facilities, and their associated utilities. (The Site 300 facility operations team will be the subject of a future article.)

Carey currently has 12 individuals working for him, keeping all those buildings humming. Patty Brooks is Carey's administrative assistant. "She keeps me organized," he says, "and she maintains a CMS locations database that records all activities in CMS spaces." Three facility coordinators, Frank Beckett, Doug Higby, and Barney Hernandez, handle requests from building residents. They arrange office moves, ready laboratories for transfer between scientists, maintain the vehicle fleet, and, most importantly, keep CMS facilities running smoothly. Material coordinators Joe Warren, Greg Brattelle, and Juan Vargas make deliveries, move and rearrange office furniture, and haul away excess materials.

Project manager **Barbara Pulliam** has directed the isotope science facility line

item project in recent years. Currently on loan to Plant Engineering as a project manager, she also continues to provide project management services to CMS. **Dave Sprayberry** oversees lab remodeling and reconfiguration projects. If you would like something done in your laboratory, Dave is the person to call. He recently completed development of the clean room in the basement of Building 235 now being used by the focused ion beam, described in an article on p. 1.

Yolanda Villa and Leslie Vigil-Wright manage the CMS property center, including the transfer and inventory of over 5,000 individual items. Yolanda is also responsible for the CMS ergonomic program. Dick Quigley is the Laboratory's "chief scrounge." When a Livermore project needs special equipment, his job is to find surplus property at other DOE or DoD sites and get it to Livermore, typically for pennies on the dollar. His biggest find to date was the huge Manatewok crane used to lift the National Ignition Facility's target chamber from its construction site and precisely place it in the NIF target bay.

Besides the day-to-day routine of maintaining all of the buildings, a number of major projects keep Carey's team busy. The most visible is the recent construction of an entirely new building, Building 155, with its modern, spacious auditorium for CMS gatherings. A seismic upgrade of Building 151 has been completed, and a seismic upgrade of Building 241 is planned soon. The heating, ventilating, and air conditioning (HVAC) system in Building 151's dissolver wing was recently upgraded as well as the HVAC system in Building 154. Other projects include replacing the chillers in Buildings 241 and 235, installing new boilers in Buildings 235 and 241, and replacing most of the air handlers in Buildings 241 and 151.

"We have a very close partnership with institutional facilities management and with Plant Engineering," says Carey. "Institutional facilities management provides funding for many of our projects, and we work hand in hand with Plant Engineering to get all the work done."

The facilities team works to keep CMS facilities and the surrounding areas safe for employees. Ergonomic evaluations have recently been completed. Computer workstations have been retrofitted with keyboard trays and foot rests, and Stretchware software has been installed. In laboratories, robotic tools and other devices help keep employees healthy. Cracks in sidewalks have been repaired where tree roots pushing up concrete had created tripping hazards.

"I believe the most important part of the facilities management job is to provide top-notch customer service," Carey says. "And I think we're doing our job best when the people who work in our buildings don't have anything to complain about." CMS facility coordinators strive to perform maintenance and make changes and upgrades to buildings with as little disruption to scientists and other building occupants as possible. Carey encourages all employees to notify his team when even minor maintenance appears to be needed. "Don't wait until things break before notifying the facility coordinators," says Carey. "Major fixes result in more disruption for everyone."



Left to right, back row: Frank Beckett, Joe Warren, Carey Bailey, Barney Hernandez, Barbara Pulliam Front row: Leslie Vigil-Wright, Patty Brooks, Doug Higby, Yolanda Villa



Awards and Personnel News

DOE Award of Excellence



Mark Lane (left) and Bryan Balazs of CMS were part of a team from Livermore and Y-12 whose work on the W80 baseline design review garnered all team members a DOE Award of Excellence. In a ceremony on August 23 in Oak Ridge, Tennessee, the team was honored for their work on an aggressive project plan for high-priority testing and evaluation. One test was a first-ever event for the

nuclear weapons complex, and the other was a first-ever event for Y-12 and only the second ever for the nuclear weapons complex. The team helped coordinate Livermore's needs and Y-12's existing and potential capabilities, determined the tests' parameters and controls, assessed the risks associated with several proposed approaches, and prepared for the appropriate risk-mitigating actions. Congratulations, Mark and Bryan!

Wayne King Is Distinguished Alumnus

Wayne King was awarded the Thiel College Distinguished Alumnus Award during an October 1 alumni awards ceremony on the college's campus in Greenville, Pennsylvania.

King, who earned a B.A. in physics and math from Thiel in 1975, serves as acting deputy division leader for science and technology in MSTD. He is leading a new effort at Livermore to construct the first transmission electron microscope in the U.S. that can acquire images with nanometer spatial resolution and nanosecond time resolution. When King joined Livermore, he launched a research project in the area of adhesion and bonding at interfaces in materials. More recently he began a research program on grain boundary engineering where techniques were developed to give ordinary materials extraordinary properties.

Thiel College's Distinguished Alumnus Award winners are nominated by their fellow alumni for outstanding contributions to their professions.



Wayne King (left) receives Thiel College's Distinguished Alumnus Award.

CMS Employees Honored with S&T Awards

On October 1, Laboratory Director **Michael Anastasio** presented the fifth annual Science and Technology Awards to two teams of Laboratory scientists.

Jerry Britten led the team that developed the processing methods and tooling that produced both the world's largest multilayer dielectric reflection grating and the world's highest laser damage-resistant gratings. This technology provides optics for highenergy, short-pulse lasers. Until this breakthrough was made, no gratings were available for any of these lasers. Fellow CMS employees on the team include James Peterson, Curly Hoaglan, and Leslie Summers.

Anthony Van Buuren was a member of the team that discovered bucky-diamond and unraveled the atomic structure of silicon and germanium nanoparticles. The team's research focuses on how the properties of materials change as they are squeezed and made smaller.

James Peterson and Jerry Britten are fourth and fifth from left. Leslie Summers and Curly Hoaglan second and third from right.





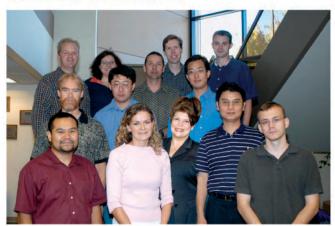
Anthony Van Buuren is second from right.

Kudos to CMS Employees from DNT

DNT recently granted awards to the following CMS employees:

- · Jackie Kenneally for the U19a drill back.
- Ken Moody and Jackie Kenneally for successfully communicating a potentially costly oversight regarding the scheduled disposition of unique and expensive radioactive tracers that are critical in maintaining an effective test readiness capability.
- · Richard Quigley for "fork trucks."
- Frank Garcia for exemplary teamwork.
- · Sally Weber for after-hours checking.
- Clark Souers for work on HE equation of state.
- Wardell Black, Pat Gallagher, Mark Hoffman, Mike Kumpf, Kirk Pederson, and Roz Swansiger for the DIME test.
- Wardell Black, Pat Gallagher, Michael Kumpf, Kirk Pederson, Roz Swansiger, and A.J. Boegel for BALSC units.
- Bryan Balazs for outstanding support of surveillance activities.
- Mark Lane for outstanding support of the W80 cold test.
- Bill McLean for outstanding support with surveillance activities.
- George E. Overturf for bringing his knowledge of the science of energetic materials to detonator aging and development.
- Adam Schwartz, Mark Wall, and Jessee Welch for work on new and aged materials.
- Lydia Hunt and Jennifer Burch for outstanding effort on documentation associated with legacy materials.
- Vasily Bulatov, Masato Hiratani, and Tom Arsenlis for their work for the ASC Team.
- Adam Schwartz and Mark Wall for building and demonstrating a plutonium coining apparatus.
- Wigbert Siekhaus who completed and applied a predictive aging model for intermetallic growth and alloy formation.
- Doug McAvoy for work on a 24/7 compressed air system.
- Don Bajao, Jennifer Burch, Andrea Goins, Lydia Hunt, Robert Klatt, Daniel Mew, and Joe Schmitz for completion of TRU drum seeding in support of DNFSB 94-1 completion milestone.
- Rich Torres for exceptional creativity in his completion of the DOE/LANL plutonium metal exchange samples project.

Welcome to the Directorate



Top row from left: Ted Tarasow, Jennifer Giocondi, Nick Teslich, Michael

Armstrong, Jon Lee

Middle row from left: Phil Norton, Kenneth Kim, Richard Kimura Bottom row from left: Saphon Hok, Amy Fierce, Karen McWilliams, Luan Nguyen, David Campbell

Not shown: Farid Abraham, Jaime Marian, Lucien Mihailescu, Kathleen Moody, Andrew Saab, Tuan Truong

So Long, Farewell, Good-Bye...

Wonyong Choe Tai-Gang Nieh

Gilbert Gallegos David Sisson Jesse Yow David Hare Bahrad Sokhansanj Loreen Zeller

Sally Hooper Maximo Victoria Kenneth Marsh Brandon Weeks Walter Martin Louisa Hope-Weeks

Postdoc People News

A big hello to these new CMS postdocs:

David Campbell (CBN) Jennifer Giocondi (CBN) Saphon Hok (CBN) Jonathan Lee (CBN)

Michael Armstrong (MSTD) Evan Reed (Lawrence Fellow)

These former postdocs are now flex-term employees:

Anthony Esposito (CBN) Sarah Chinn (CBN) Jonathan Crowhurst (CChED)

Bradley Hart (CBN) Kerri Blobaum (MSTD)

And we bid a fond farewell to these postdocs:

Stephen Glade Wonyong Choe Alexander Ziegler Wei Cai



Message from the Associate Director Continued from page 1

The BSNL was awarded more than \$4.5 million in new grants in FY04, leveraging support from a healthy mix of sponsors in both fundamental bioscience and national security applications. Not only has BSNL positioned itself as the powerhouse of bionanoscience expertise within the Laboratory, it has also quickly garnered funding from a host of national agencies, such as the National Institutes of Health, the Federal Bureau of Investigation, and the Department of Homeland Security.

Our priority for FY05 is to initiate a thrust area in optics and photonics while phasing out successful initiatives that have become largely funded by programs. This new thrust area will provide us with diagnostics and design capabilities that will underpin future research to extend optical materials for the new generation of laser technologies.

Effective Integration of Myriad Resources

Our key investment strategy is to integrate all internal funding sources—including LDRD, general and administrative (G&A), and institutional general-purpose equipment—and maximize the return on a few selected, strategic investments. A leading example is the launch of the Nanoscale Synthesis and Characterization Laboratory (NSCL) this year.

In less than a year, the NSCL has already had a major impact on the Laboratory, tackling the enormous challenges of nanomaterial synthesis, characterization, and fabrication for applications in advanced targets for NIF. Its startup involved combined resources from all major funding sources—from facility improvement to capital equipment procurement, from LDRD to G&A. The NSCL's early successes, such as the synthesis of thick diamond films, low-density nanoporous gold foam, and high-strength nanocrystalline metal, are the direct fruition of our strategic investments.

Outlook for FY05

As we move forward to the implementation phase of our strategic plan, we will identify new investment wedges that offer the most return on investment. For example, as a result of ongoing strategic discussions, the Biomolecular Imaging Center will be a centerpiece of our FY05 investments. It will consolidate five bioscience laboratories from three different buildings to the basement of Building 151, collocating the complete suite of capabilities in atomic force microscopy, chemical force spectroscopy, scanned probe imaging, nanophotonics, and fluorescence microscopy.

Although the outlook for the budget reflects systemic strains, we will continue to rely on strategic planning to invest our resources effectively. At the beginning of a new fiscal year, we are confident and more committed than ever to our increasing responsibilities as a partner and a leader in our important national security mission.

Cheers, Tomás

Media Day at the BSNL



Jim De Yoreo, director of the BioSecurity and Nanosciences Laboratory (BSNL), talks to the press at the September 23 media day for the BSNL and the Center for Biotechnology, Biophysical Sciences, and Bioengineering.

Number Theory

K. Balasubramanian

All numbers are created equal Yet some are more prime. But then why some are real And others are truly imaginary?

All numbers are created equal Yet all numbers are complex. But then why some numbers Are more rational than others?

All numbers are created equal And many numbers are integral. But then why some are positive And others are negative?

All numbers are created equal And many numbers have values. But then why there is a number That's zero like an empty tumbler?

Are there equal numbers?
Or is it only in my slumber
That I see transcendental numbers
And the eternal infinity?

This poem was inspired by a professor who made the comment that all numbers are created equal.

Corner on Science

Continued from page 1

The FIB's primary strength is in material characterization, supplying detailed information about the structure of materials in three dimensions so that its performance can be understood. The combination of the two highly focused beams creates an extraordinarily powerful instrument. Operating in a vacuum, the ion beam can remove or add material from a sample while the evolution of the sample's surface topography is imaged at very high resolution with the electron beam. The electron beam can also produce electron backscattered diffraction patterns that identify the crystalline structure of a material. Additionally, when the electron beam is used to stimulate the production of x rays from a sample, an analysis of the x rays by an energy dispersive spectrometer provides unambiguous identification and quantification of the elements that comprise the material.

An especially exciting application of the FIB will come along in 2006 when dust particles from Comet Wild 2 will arrive at the Nanobeam Precision Characterization Laboratory. NASA's Stardust spacecraft was launched in

February 1999 and flew halfway to Jupiter before it met up with the comet this past January. As Stardust flew by the comet's nucleus and through a halo of gases and dust at its head, cometary dust was collected in a grid filled with aerogel. The aerogel grid from Wild 2 will look much like the aerogel below filled with interstellar dust collected at the Mir Space Station.

Given that Stardust will deliver less than one milligram of particles to Earth in the aerogel grid, the FIB will have to hunt for particle needles in the aerogel haystack. "We'll use the electron beam



Tracks of interstellar dust collected at the Mir Space Station are shown trapped in a sample of aerogel. The focused ion beam will find and remove dust particles captured during a NASA fly-by of Comet Wild 2 when the aerogel collector arrives at Livermore in 2006.

and the x-ray microscope attachment to locate the Wild 2 dust particles buried in the aerogel," says Wall. "Then the ion beam will slowly cut away the aerogel to get down to each particle." A probe whose tip is about ten atoms wide will reach down into the aerogel and touch the particle; then the ion beam will be used to create a nanoweld between the tip and the particle. The particle will be lifted out and delivered to the SuperSTEM, where its internal structure can be examined.

The FIB's unique ability to find needles in haystacks has been exploited in the semiconductor industry for several years. When a few of the millions of integrated circuits on a silicon wafer are found to be defective, FIB can quickly find the bad spots and remove them for further characterization, saving the remainder of the expensive wafer. Similarly, nanometer-scale tolerances and precision are essential for the successful synthesis and fabrication of targets for experiments on NIF and other high-energy-density platforms. The FIB will assist with characterizing, analyzing, and repairing target components and their assemblies.

Interview With... Continued from page 1

tors and others at their alma maters to learn about the latest crop of talented, hardworking B.S., M.S., and Ph.D. grads. Pat's recruiting responsibilities also extend beyond NIF and include finding exceptional postdocs, some of whom eventually become full-time employees. Web-based ads, trade journals, and national meetings have also proved helpful for recruiting top talent across the CMS core disciplines.

For getting people interested in energetic materials, another of CChED's core areas, Pat says, "The Energetic Materials Center's student program is excellent. We had eight students participate this past summer and expect to have a similar number next year." Pat greatly enjoys mentoring students and postdocs.

Pat received his B.S. in chemistry from the University of Cincinnati and his Ph.D. in physical chemistry from the University of Michigan. He arrived at Lawrence Livermore in 1998, by way of both Lawrence Berkeley and Los Alamos national laboratories. Since coming to Livermore, he has worked as a scientist and later served as deputy director of the Glenn T. Seaborg Institute, where he focused on basic actinide

chemistry research. In October 2003 he became deputy division leader for CChED.

Throughout Pat's career, extended x-ray absorption fine structure (EXAFS) spectroscopy has been his specialty. Pat has used EXAFS, an excellent tool for examining structure at the molecular level, to study plutonium and other actinide elements. Many of his experiments have been conducted at the Stanford Synchrotron Radiation Laboratory, and Pat has served as chairman of the SSRL users committee.

Almost immediately after Pat accepted his current position, physicist **Bruce Remington** approached him about collaborating as the EXAFS data expert for a series of experiments on the Omega laser at the University of Rochester. Remington's team is studying phase transitions in titanium and iron at the high pressures and strain rates induced by laser-driven shock waves. Pat will also be part of a project recently funded by the DOE's Office of Basic Energy Research to study the structure and properties of plutonium and other transuranic compounds. "I really like being deputy division leader but still being able to do some science is great," he says. **•**



Laboratory Directed Research and Development at CMS

A contributor in LDRD: Sarah Chinn



As a freshman at Mt. Holyoke College, **Sarah Chinn** intended to study biology and become a veterinarian. Instead, Sarah became so intrigued by her introductory chemistry classes that she shelved her original plans, switched her major to chemistry, and went on to pursue a Ph.D. in physical chemistry at UC Davis.

After one of Sarah's fellow Ph.D. students became a CMS postdoc, he introduced Sarah to **Bob Maxwell**, the scientific capability leader for CMS's nuclear magnetic resonance (NMR)

group. Bob later invited Sarah to join CMS, and she began a postdoctoral appointment in July 2002. She became a full-time Laboratory employee precisely two years later.

Sarah has been part of CMS's Center for National Security Applications of Magnetic Resonance (CNSAMR) since arriving at the Laboratory. She is an active participant in

three LDRD projects. In a joint CMS-DNT project, Sarah is working with CMS scientists **Ted Baumann** and **Joe Satcher** and using NMR to characterize aluminum aerogels that will be in targets for National Ignition Facility experiments. The goal of the project is predictive synthesis of these advanced aerogels.

"NIF experimenters would like to be able to produce the aerogels with specific, tailorable properties," Sarah says. Sarah's team is using NMR to follow the gelation process over time. When an aerogel sample is placed in NMR's magnetic field, a newly developed probe produces signals that allow Sarah to measure the morphology of the sample as it moves from a liquid state to a gel and on to a solid. As data is collected on many varied samples, the goal of dictating an aerogel's precise properties during synthesis becomes more feasible.

Two other LDRD projects are collaborative efforts with scientists from the Center for Accelerator Mass Spectrometry. Both projects are investigating carbon sequestration, one in soils and the other in ocean sediments. Sarah is using solid-state NMR to reveal how carbon is stored in these materials: what types of carbon are being held, how they are being stored, and what is being released.

Sarah enjoys the Laboratory's dynamic environment, the mix of academic and applied work, and the many collaborative opportunities to participate in "amazing science." She also deeply appreciates the strong team environment at CNSAMR and is an advocate for women in science.

Conference Calendar

DATE	CONFERENCE	LOCATION	WEB SITE	
November 29– December 3, 2004	Materials Research Society Fall Meeting	Boston, MA	http://www.mrs.org/meetings/ fall2004/index.html	
November 14–19, 2004	The American Vacuum Society 51st International Symposium	Anaheim, CA	http://www2.avs.org/call/ default.asp	
March 13–17, 2005	229th American Chemical Society National Meeting	San Diego, CA	http://www.chemistry.org/portal/ a/c/s/1/acsdisplay.html?DOC= meetings\sandiego2005\sa05_ index.html	

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